Quantitatively Accurate Simulation of Quantum Semiconductor Devices

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Abstract

The quantum well resonant-tunneling diode has attracted a good deal of attention over the past few years, primarily because the active region of this device spans such a small length. Simplified quantum-mechanical models of this device abound, but these have been unsuccessful in quantitatively describing the device characteristics. We have found that agreement with experimental characteristics can be markedly improved by using more realistic energy-band and potential profile models.

1 Introduction

Efforts to realize useful quantum devices have resulted in the investigation of a multitude of different material systems. The proliferation of exotic material systems has placed many demands on theorists trying to predict quantum transport behavior in these devices. In order to model quantum transport, it is necessary to include all of the relavent states which carriers may occupy. The quantum states in a crystal are described by its energy-momentum dispersion relationship or bandstructure. The majority of theoretical investigations of quantum devices to date have employed highly simplified models of bandstructure. However, it has become apparent that a more complete description of bandstructure must be incorporated into the transport models if we are to simulate many of the promising material systems which are currently under investigation. However, full bandstructure models require the inclusion of transverse basis states in the Hamiltonian making I-V simulations numercally prohibitive. The predominant obstacle in performing such calculations is the integration over extremely narrow spectral features arising from transmission resonances.

A second issue in the simulation of these devices concerns the potential profile, and its effects on both the spectroscopy and statistics of the system. We have found that the potential profile may often be adequately described by the Thomas-Fermi (zero current) approximation, but the distribution and occupation of the states in the regions adjacent to the quantum well structure must be accurately accounted for in the calculation.

2 Energy Band Model

For several years now it has been recognized that the effective-mass model is insufficient to accurately describe tunneling through indirect gap barriers [1, 2, 3, 4]. The interaction between quasi-bound X states in the barrier with continuum Γ states results in resonance-antiresonance

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features known as Fano resonances [5]. Such features have been observed experimentally as negative differential resistance in $GaAs/AlAs/GaAs$ single barrier heterostructures [6]. In order to describe tunneling in these structures one must use models which take material bandstructures into account. In this work we choose to describe bandstructure using tight binding models. The Quantum Transmitting Boundary Method (QTBM) is implemented to obtain open system boundary conditions for the tight-binding Hamiltonian. Using this method one obtains scattering states by simply solving a sparse system of linear equations.

In order to accurately model the electronic structure of the material we have employed the $sp3s^*$ empirical tight-binding model [7]. In this basis the Schrödinger equation is expressed as:

$$H\Psi_j = -S_j^\dagger \Psi_{j-1} + D_j \Psi_j - S_{j+1}\Psi_{j+1} = E\Psi_j \quad (1)$$

Ψ_j is a subvector containing the atomic orbital coefficients for the jth layer. The Hamiltonian matrix elements are contained in the submatrices S_j and D_j. The tight-binding parameters used in this work are taken from Boykin [8]. In our formulation each layer corresponds to a lattice unit cell. Therefore these subvectors and submatrices are of order ten for the $sp3s^*$ model (5 anion and 5 cation orbitals). At the GaAs/AlAs interface the tight binding parameters are taken to be the average of those in the bulk materials on either side.

This Hamiltonian is coupled to the semi-infinite contact regions by adapting the Quantum Transmitting Boundary Method (QTBM) [9, 10] to the tight binding basis. The QTBM operator is equivalent to the inverse of the propogator (g^r) for the system. We have developed efficient numerical techniques to locate the poles and zeros of g^r Our approach is to determine the position and width of the resonance lineshape by numerically locating the poles of the propogator $g^R(E)$ in the complex energy plane. We have developed a shift and invert non-symmetric Lanczos algorithm which allows us to rapidly determine the location of these poles [11]. The complex energies associated with the poles provides the location and width of the sharp features in the transmission coefficient. With this information we may obtain an analytic fit to the transmission characteristic. In order to obtain the fit, we assume a rational form for the transmission lineshape and expand the denominator as a partial fraction.

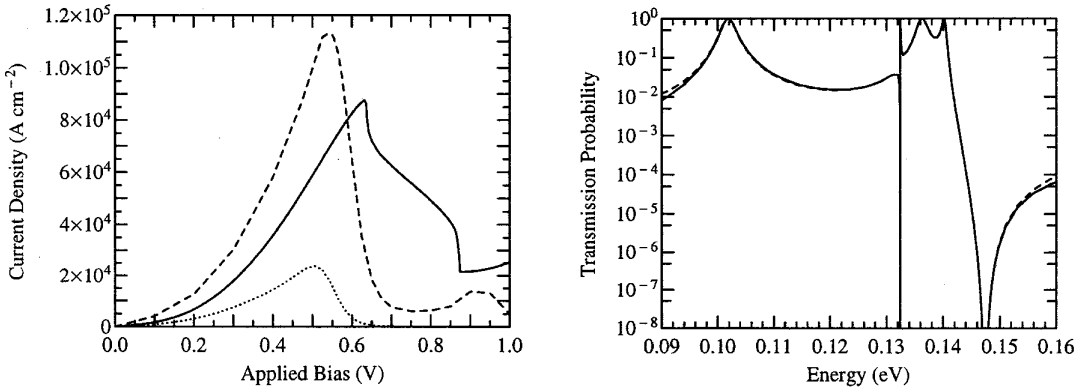
$$\begin{aligned} t(E) &= \frac{\prod_i (E - E^z{}_i)}{\prod_j (E - E^p{}_j)} \\ &= \left[\prod_i (E - E^z{}_i)\right] \left[\sum_j \frac{R_j}{(E - E^p{}_j)}\right] \quad (2) \end{aligned}$$

Here, E^p and E^z represent the location of the poles and zeros of $g^R(E)$. The partial fraction expansion coefficients (R_j) are treated as fitting parameters for the transmission lineshape. Once the fits are obtained, integration over the resonances becomes a trivial numerical task.

We apply our method to calculate current density versus voltage in a GaAs/AlAs resonant tunneling diode. In this structure, resonances due to states confined by the X-point conduction band profile significantly contribute to the current flowing through the device. In addition, nonparabolicity of the imaginary bands in the AlAs barrier result in increased tunneling current in the device. Thus, a full bandstructure model is necessary to accurately simulate current in this structure. In Figure 1, single band and multi-band simulations of the I-V characteristic of a GaAs/AlAs RTD are compared with experiment. In Figure 2, the electron density of states arising from the single band and multi-band models are compared.

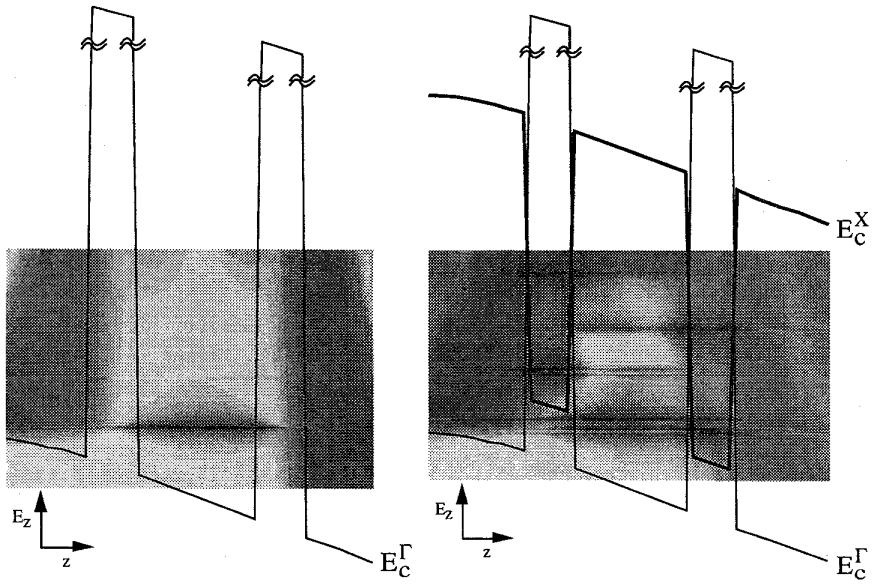
3 The Potential Profile

A critical aspect of the problem of accurately modeling resonant-tunneling devices concerns the potential profile and its effect on the density and occupation of states in the contacting layers adjacent to the quantum-well structure, as well as its effect on the transmission amplitudes through that structure. Our investigations indicate that confined states often form in the potential "notch" before the first energy barrier, and



(a) (b)

Figure 1: (a) Current density vs. voltage for a GaAs/AlAs double barrier resonant tunneling diode. Solid line is experimental data, dashed line is a full bandstructure calculation, and dotted line is a single band effective mass calculation. (b) Analytic fit for several resonances in the GaAs/AlAs double barrier resonant tunneling diode. Solid line is the actual transmission characteristic, dashed line is the analytic fit.



(a) (b)

Figure 2: (a) Single band density of states for the GaAs/AlAs RTD. (b) Multi-band density of states for the GaAs/AlAs RTD. The full bandstructure model predicts additional resonances due to states confined by the X-point profile. This results in the additional current predicted in Figure 1(a).

that tunneling of electrons out of these states is a major contributor to the peak current density [12].

The influence of such states may be efectively computed by conceptually dividing the device model into five regions:

1. The left-hand lead, a semi-infinite region in which the potential is constant.
2. The left-hand contact layer, a finite region in which the potential is determined self-consistently.
3. The quantum-well structure.
4. The right-hand contact layer, again a finite region in which the potential is determined self-consistently.
5. The right-hand lead, again a semi-infinite region in which the potential is constant.

Regions 2 and 4 are taken to be in equilibrium with regions 1 and 5, respectively. The $g^R(E)$ in each region is evaluated, including the coupling to the adjacent regions. From this quantity the (local) density of states is obtained. Invoking the local-equilibrium assumption in regions 2 and 4 then produces the charge density in these regions by integrating the occupied-state density with respect to energy. The charge density in region 3 may be neglected in most devices (except those designed to emphasize intrinsic bistability). The self-consistent potential profile is then readily obtained by iteration. The tunneling current is evaluated only across region 3, but this is done by taking into account the density of states and occupation in regions 2 and 4.

In effect, this procedure presumes that there is a high rate of inelastic processes within regions 2 and 4. (Quasi-equilibrium is maintained if the rate of inelastic collisions in these regions is significantly larger than the rate of carrier loss by tunneling.) Inelastic processes which occur during the tunneling processes are of course also of interest. Lake and co-workers have developed techniques required to treat such processes within the nonequilibrium Green's function (or Keldysh) approach [13]. Their results indicate that the inclusion of such processes usually has a much less pronounced effect on the $I(V)$ curve than the band structure and potential profile effects emphasized here.

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